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MEAN LIFE OF THE $2p^4(^1S)3s\ ^2S$ STATE IN FLUORINE

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In the emission spectrum of atomic fluorine, Liden¹ observed two lines above the first ionization limit at 680.7 and 682.6Å, and assigned them to be the transitions from the $2p^4(^1D)4s\ ^2D$ upper state to the $2p^5\ ^2P_{3/2,1/2}$ ground states. However, these two lines were not seen in the absorption spectrum of Huffman et al.² Instead, two lines at 681.8 and 683.7Å appeared. The upper state was re-interpreted by Palenius^{3,4} as the $2p^4(^1S)3s\ ^2S$ state, which is forbidden to autoionize in the LS coupling limit and can thus give rise to emission lines above the ionization limit. As for the $2p^4(^1D)4s\ ^2D$ state which is allowed to autoionize, it was assigned to the observed absorption lines instead.

Recently, in the photoionization spectrum of fluorine by Ruscic et al.,⁵ a strong peak shows up at 680.7Å. This is rather surprising because such a strong peak should not appear at all if the $2p^4(^1S)3s\ ^2S$ state is forbidden to autoionize. A logical explanation is that the autoionization rate of this state, though suppressed, is still comparable in size to the radiative decay rate. This is possible by a break down of the LS coupling due to the spin-orbit interaction. Berry et al.⁶ have since measured the life time of this state with a beam-foil technique. Comparing their result with the theoretical radiative life time by Cheng⁷ and that by Beck,⁸ they deduce that the autoionization rate is at least three times higher than the radiative decay rate. However, there is as yet no direct study of the branching ratio between the two decay mechanism.

In this work, we calculate the radiationless as well as the radiative decay rates for the $2p^4(^1S)3s\ ^2S$ state. For comparison purposes, we also make similar calculations for the $2p^4(^1D)4s\ ^2D$ state. Our calculation is based on the multi-configuration Dirac-Fock (MCDF) method. As spin-orbit interaction is built in, this method is capable of studying LS forbidden Auger transitions. Details of the Auger transition calculations have been given before.⁹

Results of our calculations are given in Table I. As one can see, while the forbidden Auger rate is about two orders of magnitude smaller than the allowed one, it is still almost one order of magnitude higher than the radiative decay rate, indicating that the spin-orbit interaction is indeed quite strong for neutral fluorine. Resulting theoretical life time for the $2p^4(^1S)3s\ ^2S$ state is consistent with the experimental result of Berry et al.⁶ Also shown in Table I are the absorption oscillator strengths from the $2p^5\ ^2P_{3/2}$ ground state, which also agree well with the values determined from the fluorine spectrum of Ruscic et al.⁵ Details of our present calculation will be published as a separate paper.

TABLE I. Decay rates (in sec^{-1}), life times (in nsec) and absorption oscillator strengths from the $2p^5\ ^2P_{3/2}$ ground state (f) for the $2p^4(^1S)3s\ ^2S$ and the $2p^4(^1D)4s\ ^2D$ states of fluorine

	$2p^4(^1S)3s\ ^2S$	$2p^4(^1D)4s\ ^2D$
Auger rate	4.6×10^9	2.5×10^{11}
Radiative rate ^a	5.1×10^8	6.6×10^7
Total rate	5.1×10^9	1.5×10^{11}
Life time	0.2	0.004
Life time (expt) ^b	0.31 ± 0.10	
f	0.012	0.009
f (expt) ^c	$0.019^{+0.011}_{-0.005}$	$0.010^{+0.005}_{-0.004}$

^aInclude decay rates to the $2p^5\ ^2P_{3/2,1/2}$ ground state only

^bBerry et al, Ref. 6.

^cRuscic et al, Ref. 5.

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REFERENCES

1. K. Liden, Ark. Fys, 1, 229 (1950).
2. R. E. Huffman, J. C. Larrabee and Y. Tanaka, J. Chem. Phys. 47, 846 (1967).
3. H. P. Palenius, Ark. Fys. 39, 425 (1969).
4. H. P. Palenius, R. E. Huffman, J. C. Larrabee and Y. Tanaka, J. Opt. Soc. Am. 68, 1564 (1978).
5. B. Ruscic, J. P. Greene and J. Berkowitz, J. Phys. B17, L79 (1984).
6. H. G. Berry, L. P. Somerville, L. Young and W. J. Ray, J. Phys. B17, 3857 (1984).
7. K. T. Cheng, unpublished results quoted in Ref. 6.
8. D. R. Beck, unpublished results quoted in Ref. 6.
9. M. H. Chen, Phys. Rev. A31, 1449 (1985).

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